## §14. Molecular Dynamic Simulation of Static and Dynamical Properties of Point Defects in Ceramic Materials

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Ionic crystals have their own characteristics, such as good electric insulation and heat resistance, and they have become increasingly important for fission and fusion reactors. The microstructural evolution of ionic crystals under radiation fields is based on the displacement process of atoms and the subsequent kinetic process of point defects. In order to understand fundamental properties, such as the formation ($E_f$) and the migration ($E_m$) energy of Frenkel defects, the stable configuration of defect clusters and the nucleus of interstitial loops, a molecular dynamic (MD) simulation code is constructed. Calculated results are compared with the experimental results.

The MD method consisits in the Newtonian equations of a set of n (n=1000～8000) atoms. The interatomic potential for ionic crystals is generally expressed by the following equation,

$$\phi(r) = \frac{Z_1 Z_2}{r} e^2 + A \exp\left(-\frac{r}{\rho}\right) - \frac{C}{r^6} \quad , \qquad (1)$$

where $Z_1$ and $Z_2$ are the charge of cations and anions and A, ρ and C are constants. In the present calculation, Catlow's and Sangster's potentials[1] were adopted for MgO. In order to take the long-rang Coulomb interaction into account, the periodic boundary condition and the Ewald method were also adopted.

Table 1 shows the migration energy ($E_m$), the number of recombination sites and the relaxation volume of $Mg^{2+}$ and $O^{2-}$ vacancies and interstitals together with the formation energy ($E_f$) of di-valent Mg and O Frenkel pairs. The calculations were performed for crystal I (I) and crystal II (II) that include 1000 and 4096 ions, respectively, based on the Catlow (C) or the Sangster (S) potential. The results based on experiments[2] are also shown for the comparison.

Table 1. The values of $E_m$, number of recombination sites, relaxation volume and $E_f$.

| | $E_f$ | $E_m$ | | Number of recombination sites | Relaxation volume (at.vol.) | Potential & Crystal size |
|---|---|---|---|---|---|---|
| | | Vacancy | Interstitial | | | |
| Mg | 13.11 | 1.98 | < 0.1 | 60 | | C - I |
| | 13.56 | 2.05 | < 0.1 | 56 | | S - I |
| | 13.21 | 2.12 | < 0.1 | 56 | | S - II |
| O | 12.65 | 1.97 | < 0.1 | 52 | 1.086 | C - I |
| | 13.36 | 1.99 | < 0.1 | 50 | 1.092 | S - I |
| | 13.10 | 2.05 | < 0.1 | 50 | 1.092 | S - II |
| | | 2.03±0.17 [2] | 0.05 [2] | | 1±0.8 | Experimental |

Figure 1 shows a stable configuration of a tetra-interstitial cluster which consists of two $Mg^{2+}$ and two $O^{2-}$ interstitials. In this figure, four interstitial ions introduced make four <001> type mixed dumbbells with ions on the normal lattice, and three of them are in between the nearest {110} planes. Those stoichiometric clusters in between {110} planes might grow to form 1/2<110> type interstitial loops on {110} planes, which were experimentally confirmed [2].

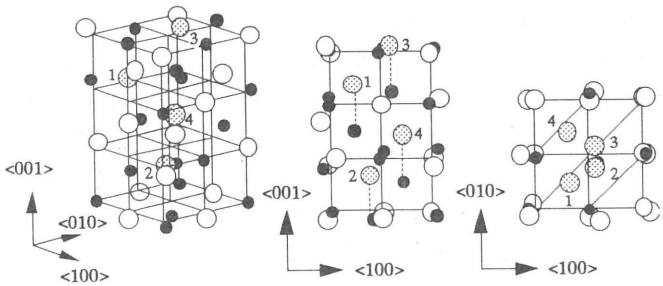


Fig. 1. A typical stable configuration of a tetra-interstital cluster and its projection onto the (010) and the (001) planes.

References

1)Sangster M.J.L and Stoneham A.H., Phil. Mag. B, Vol,43 No4 (1981) 597-608.
2) Kinoshita C., Hayashi K. and Mitchell T.E., Adv. Ceram. 10 (1984) 490.